

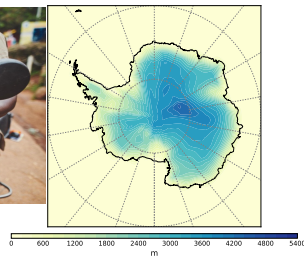
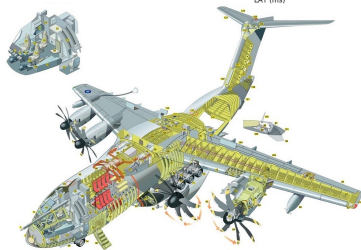
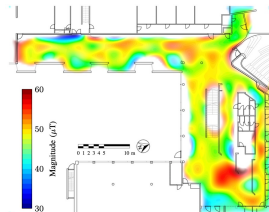
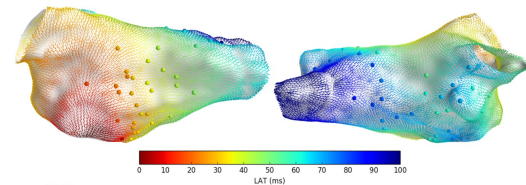
A second introduction to Gaussian Processes

Richard Wilkinson

School of Mathematical Sciences
University of Nottingham

GP summer school
September 2026

Recent GP Applications



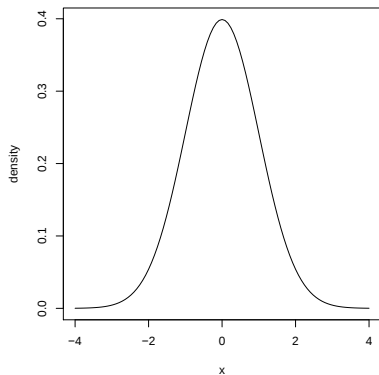
Introduction

- (Multivariate) Gaussian distributions
- Definition of Gaussian **processes**
- Motivations and derivations
- Difficulties

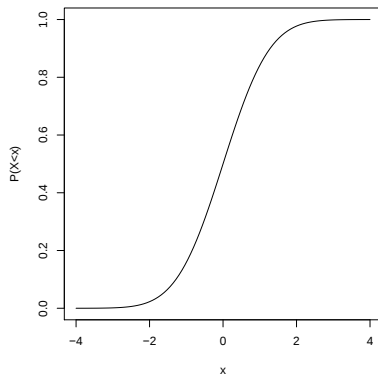
You can download a copy of these slides from www.gpss.cc

Univariate Gaussian distributions

PDF of a $N(0,1)$ random variable



CDF of a $N(0,1)$ random variable



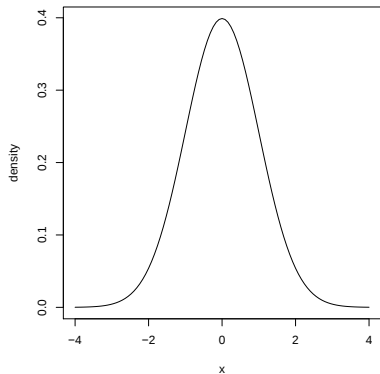
$$Y \sim N(\mu, \sigma^2)$$

PDF:
$$f_Y(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$

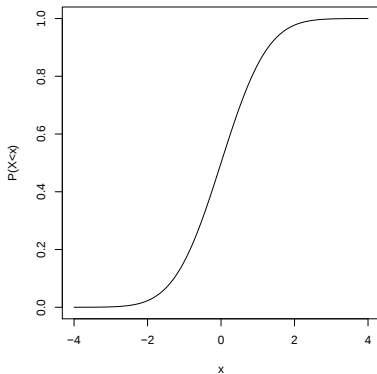
CDF:
$$F_Y(y) = \mathbb{P}(Y \leq y) \text{ not known in closed form}$$

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If $Z \sim N(0,1)$ then $Y = \mu + \sigma Z \sim N(\mu, \sigma^2)$

Univariate Gaussians

The normal/Gaussian distribution occurs naturally and is convenient mathematically

¹max. ent. principle: the distribution with the largest entropy should be used as a least-informative default

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- If Y and Z are jointly normally distributed and are uncorrelated, then they are independent
- Square-loss functions lead to procedures that have a Gaussian probabilistic interpretation
eg Fit model $f_\beta(x)$ to data y by minimizing $\sum (y_i - f_\beta(x_i))^2$ is equivalent to maximum likelihood estimation under the assumption that $y = f_\beta(x) + \epsilon$ where $\epsilon \sim N(0, \sigma^2)$.

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'Multivariate' = two or more random variables

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Suppose $Y \in \mathbb{R}^d$ has a multivariate Gaussian distribution with

- **mean vector** $\mu \in \mathbb{R}^d$
- **covariance matrix** $\Sigma \in \mathbb{R}^{d \times d}$.

Write

$$Y \sim N_d(\mu, \Sigma)$$

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Bivariate Gaussian: d=2

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \quad \mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{21}\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

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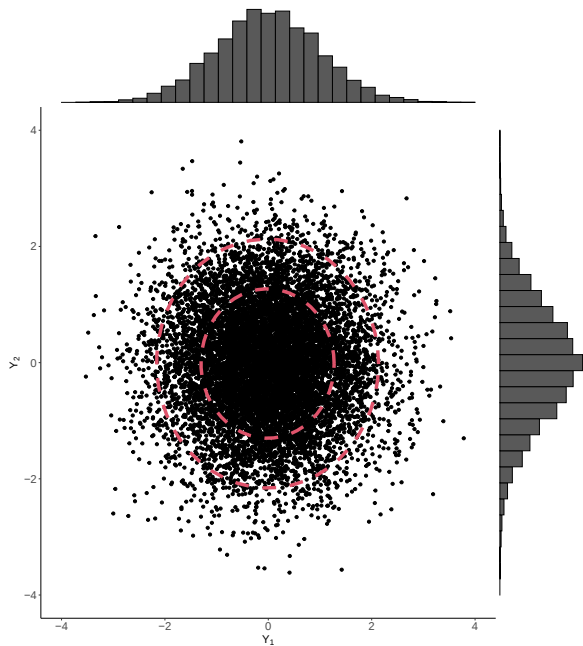
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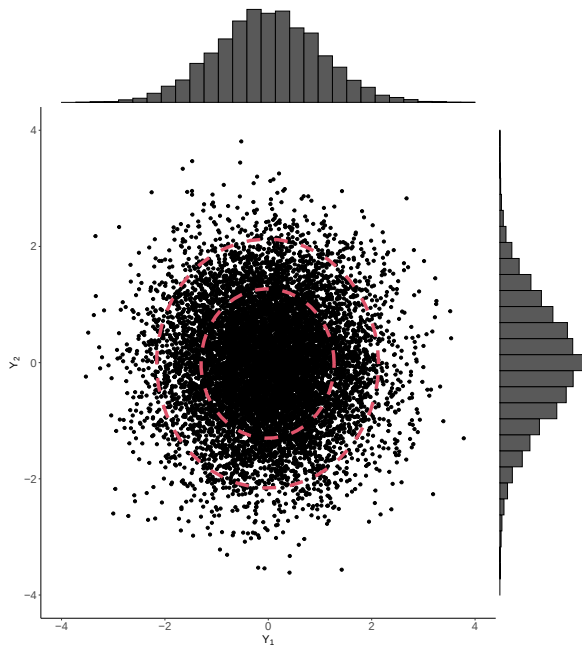
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$$\text{pdf: } f(y \mid \mu, \Sigma) = |\Sigma|^{-\frac{1}{2}} (2\pi)^{-\frac{d}{2}} \exp \left(-\frac{1}{2} (y - \mu)^\top \Sigma^{-1} (y - \mu) \right)$$

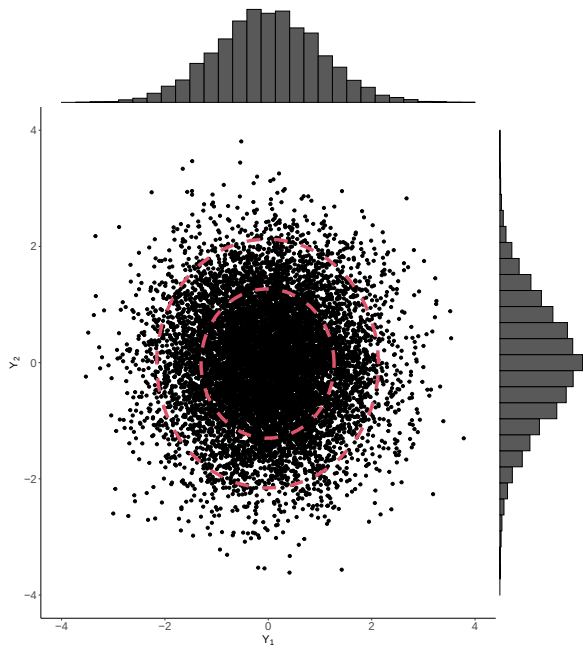


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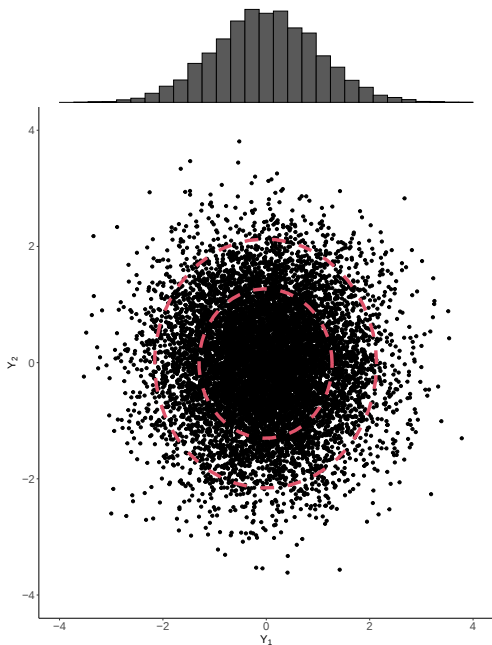
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hence Y_1
independent of Y_2



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Marginal
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 $Y_1 \sim N(0, 1)$
 $Y_2 \sim N(0, 1)$



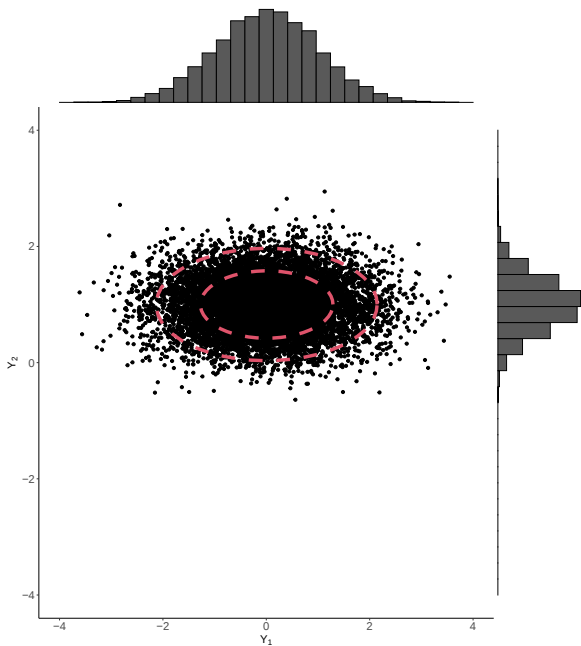
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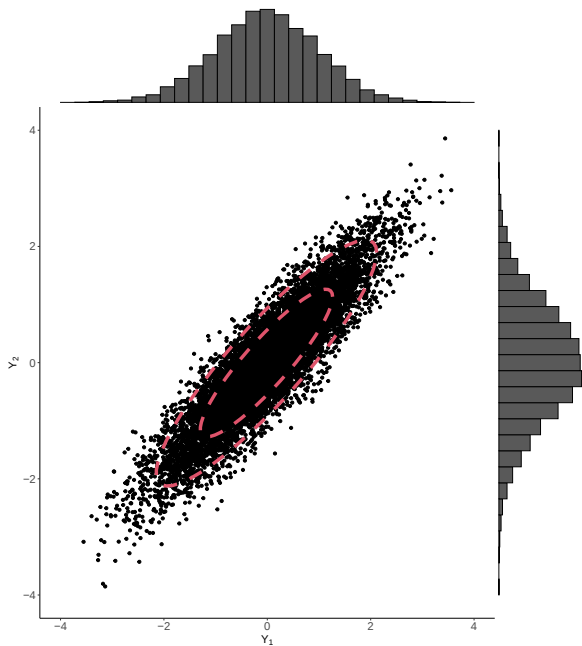
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Conditional
distributions:
 $Y_1|Y_2 \sim N(0, 1)$
 $Y_2|Y_1 \sim N(0, 1)$

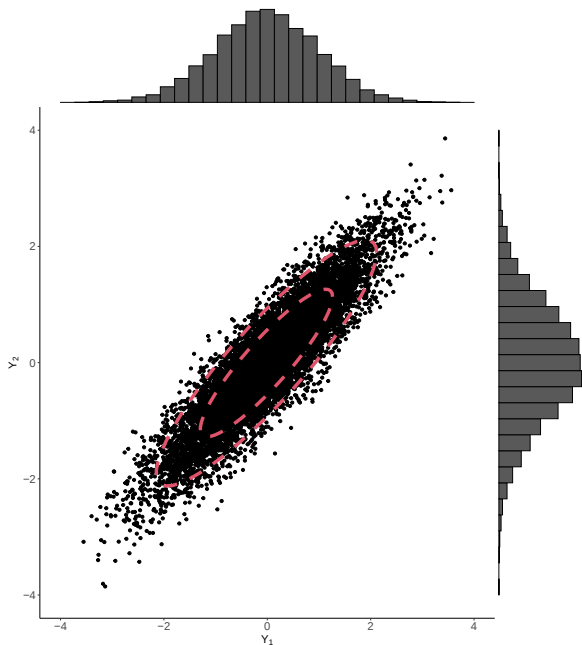


$$\mu = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 0.2 \end{pmatrix}$$

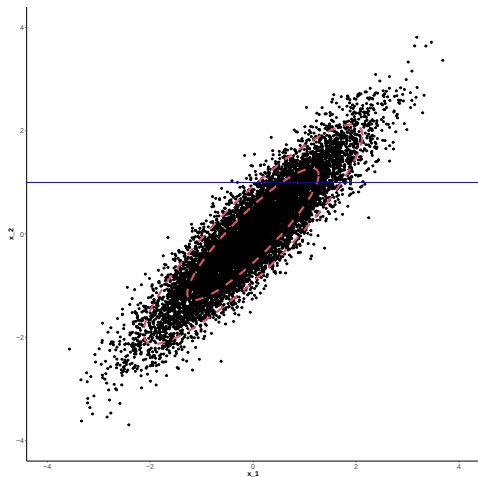


$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$\Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$



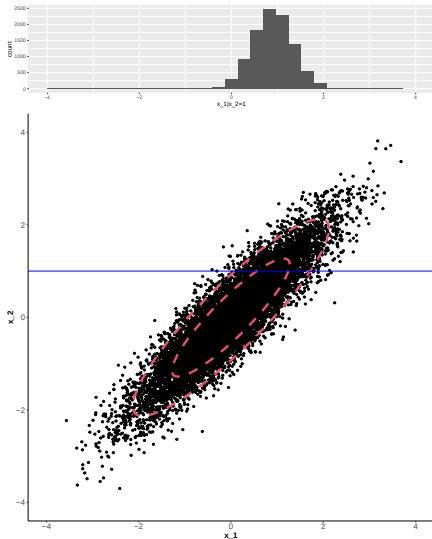
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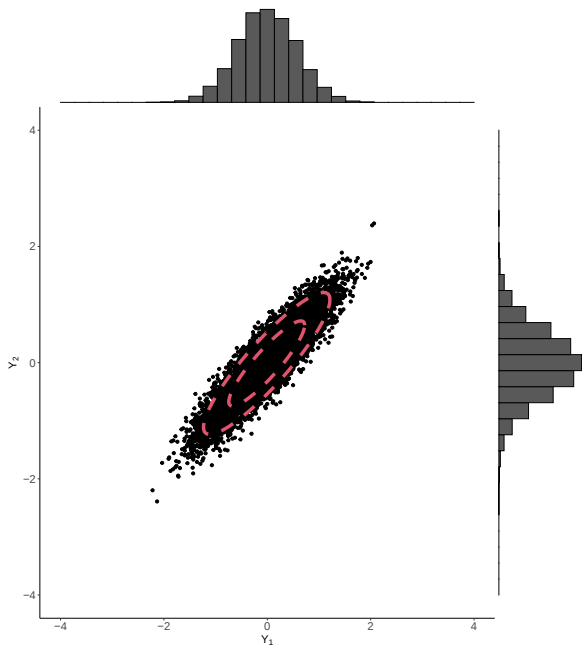
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What is the
conditional
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 $Y_1|Y_2 = 1$?



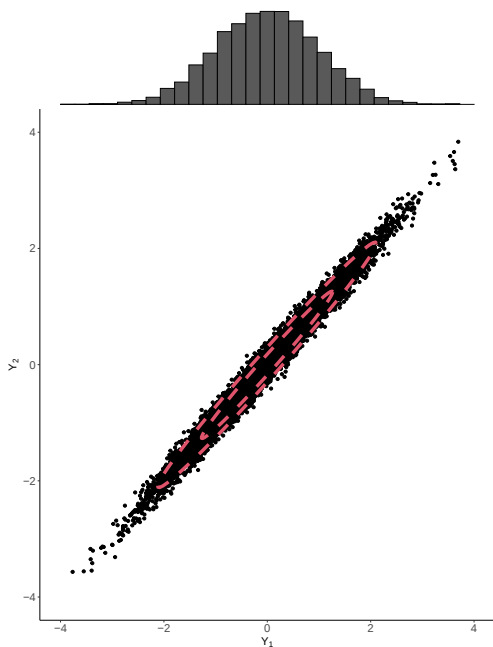
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$
$$\Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$

$$Y_1 | Y_2 = 1 \sim N(0.9, 0.19)$$



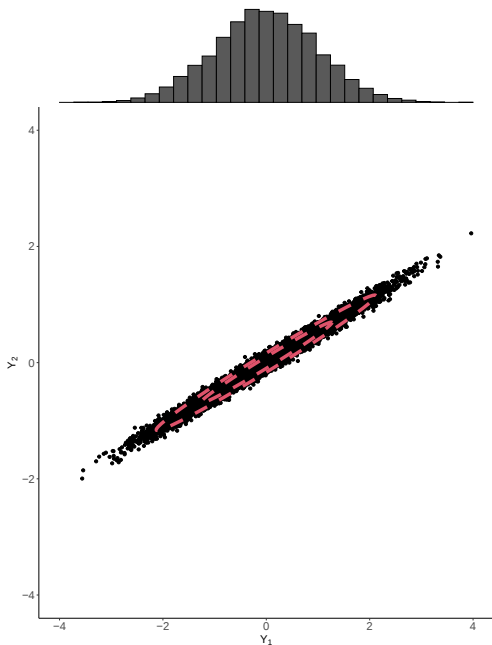
$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \frac{1}{3} \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$



$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.99 \\ 0.99 & 1 \end{pmatrix}$$



$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} 1 & 0.54 \\ 0.54 & 0.3 \end{pmatrix}$$

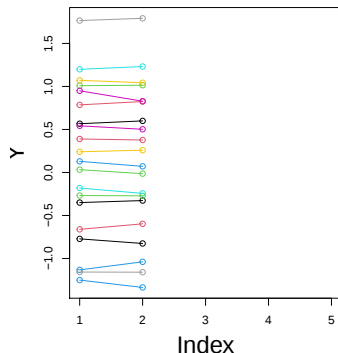
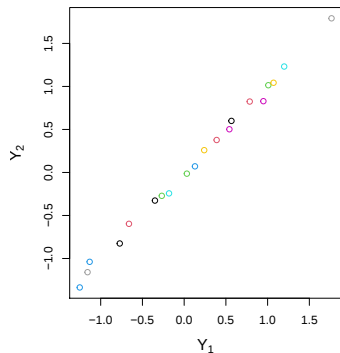
$$\begin{aligned} \text{Cor}(Y_1, Y_2) &= \\ 0.54 / \sqrt{0.3} &= \\ 0.99 \end{aligned}$$

More pictures

Hard to visualise in dimensions > 2 , so stack points next to each other.

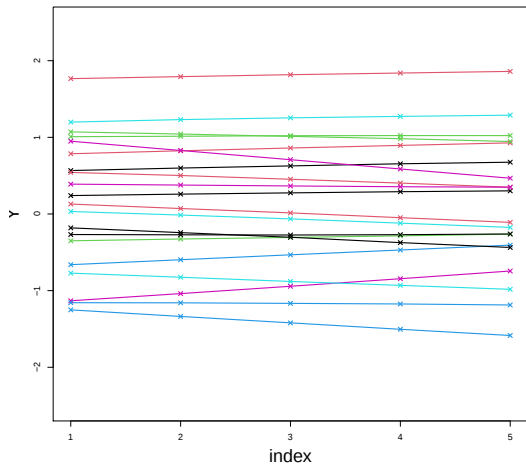
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Hard to visualise in dimensions > 2 , so stack points next to each other.
So for 2d instead of we have



Consider $d = 5$ with

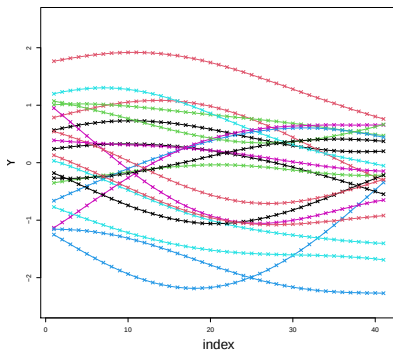
$$\mu = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 1 & 0.99 & 0.98 & 0.97 & 0.96 \\ 0.99 & 1 & 0.99 & 0.98 & 0.97 \\ 0.98 & 0.99 & 1 & 0.99 & 0.98 \\ 0.97 & 0.98 & 0.99 & 1 & 0.99 \\ 0.96 & 0.97 & 0.98 & 0.99 & 1 \end{pmatrix}$$



Each line is one sample.

$d = 50$

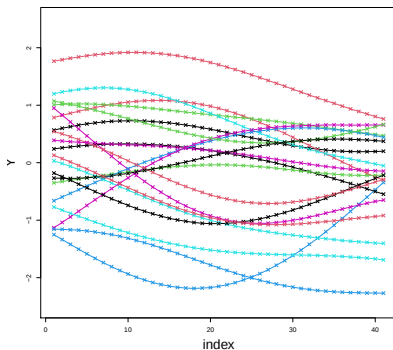
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Each line is one sample.

We can think of Gaussian processes as an infinite dimensional distribution over functions - all we need to do is change the indexing

- We can let the index be x and let x take values in $\mathbb{R}$.

Gaussian processes

A stochastic process is a collection of random variables indexed by some variable $x \in \mathcal{X}$

$$y = \{y(x) : x \in \mathcal{X}\}$$

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Thankfully, the law of y is uniquely determined by the finite dimensional distributions (FDDs), i.e., for all $x_1, \dots, x_n$ and for all $n \in \mathbb{N}$

$$\mathbb{P}(y(x_1) \leq c_1, \dots, y(x_n) \leq c_n)$$

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Write $y(\cdot) \sim GP$ to denote that we model the *function* y as a GP.

Mean and covariance function

To fully specify the law of a Gaussian *distribution* we only need the mean and variance.

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where

$$\begin{aligned}\mathbb{E}(y(x)) &= m(x) \\ \text{Cov}(y(x), y(x')) &= k(x, x')\end{aligned}$$

Specifying the mean function

We are free to choose the mean $m(x) = \mathbb{E}(y(x))$ and covariance $k(x, x') = \mathbb{Cov}(y(x), y(x'))$ functions however we like (e.g. trial and error), subject to some 'rules':

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- We can use any mean function we want:

$$m(x) = \mathbb{E}(y(x))$$

Most popular choices are $m(x) = 0$ or $m(x) = \text{const}$ for all x , or $m(x) = \beta^\top x$

Covariance functions

We usually use a covariance function that is a function of the indexes/locations

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k must be a **positive semi-definite function**, i.e., lead to valid covariance matrices:

- Given locations $x_1, \dots, x_n$, the $n \times n$ Gram matrix K with $K_{ij} = k(x_i, x_j)$

$$\begin{pmatrix} k(x_1, x_1) & k(x_1, x_2) & \dots & k(x_1, x_n) \\ \vdots & & & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \dots & k(x_n, x_n) \end{pmatrix}$$

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- This can be problematic...
 - Difficult to create semi-definite functions $k(x, x')$

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The covariance function determines the *nature* of the GP.

- k determines the hypothesis space/space of functions

We often assume k is a function of only the distance between locations

$$\mathbb{C}\text{ov}(y(x), y(x')) = k(x - x')$$

which results in a **stationary** process.

If $\mathbb{C}\text{ov}(y(x), y(x')) = k(\|x - x'\|)$ the covariance function is said to be **isotropic**.

The covariance function determines the *nature* of the GP.

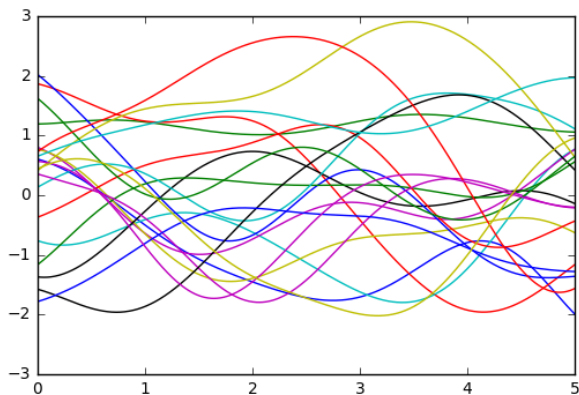
- k determines the hypothesis space/space of functions

We usually build k by selecting from a small candidate set of functions (that contain free parameters), and modifying them according to some rules.

Examples

RBF/Squared-exponential/exponentiated quadratic

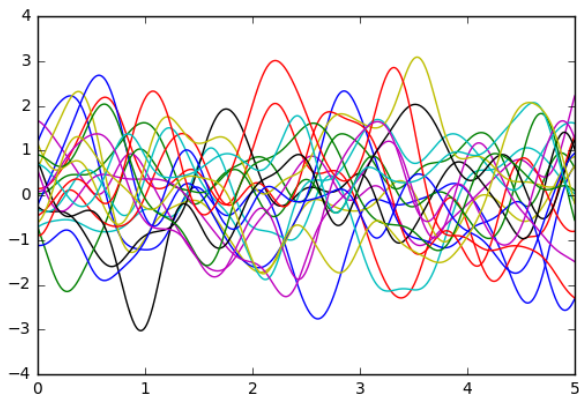
$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$



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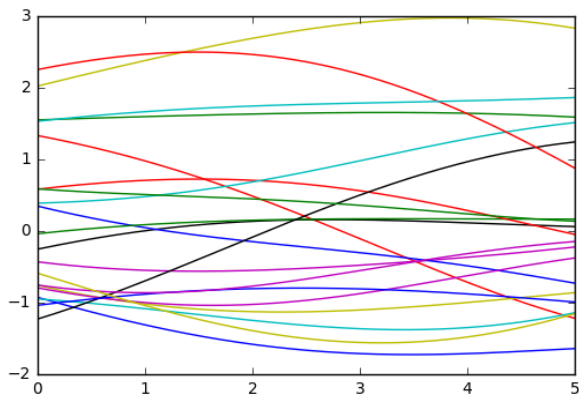
$$k(x, x') = \exp \left(-\frac{1}{2} \frac{(x - x')^2}{0.25^2} \right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

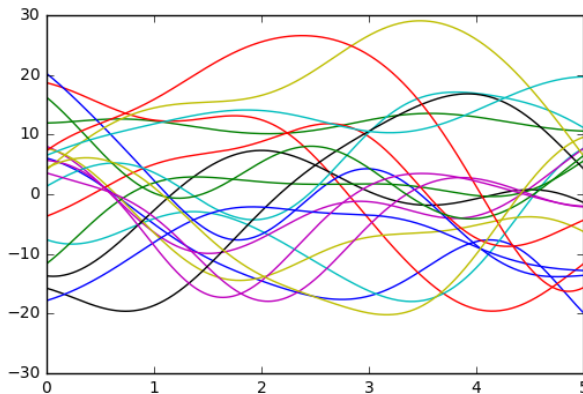
$$k(x, x') = \exp\left(-\frac{1}{2} \frac{(x - x')^2}{4^2}\right)$$



Examples

RBF/Squared-exponential/exponentiated quadratic

$$k(x, x') = 100 \exp \left(-\frac{1}{2} (x - x')^2 \right)$$

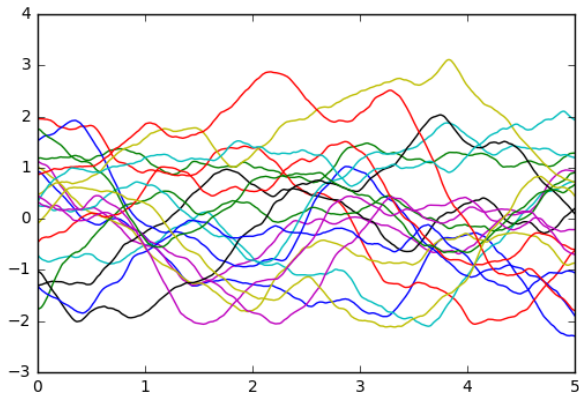


In general $k(x, x') = \tau^2 \exp \left(-\frac{1}{2} \frac{(x - x')^2}{\lambda^2} \right)$

Examples

Matern 3/2

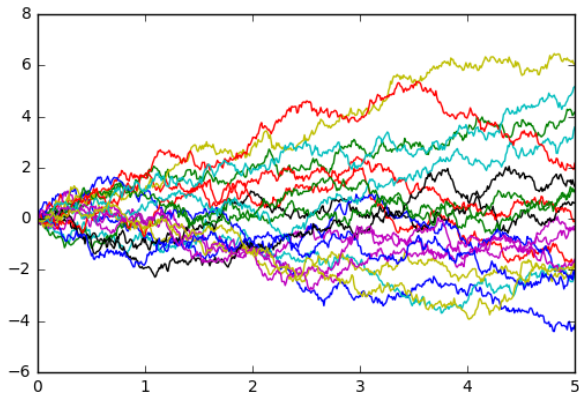
$$k(x, x') \sim (1 + |x - x'|) \exp(-|x - x'|)$$



Examples

Brownian motion

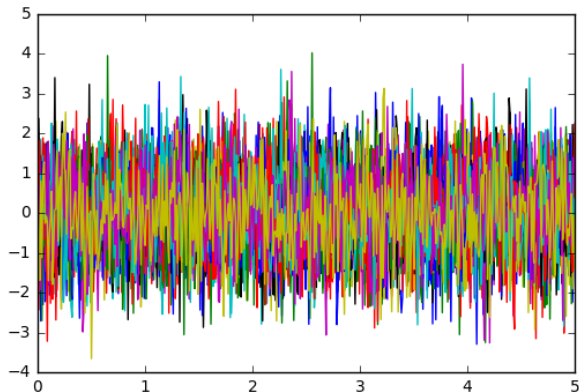
$$k(x, x') = \min(x, x')$$



Examples

White noise

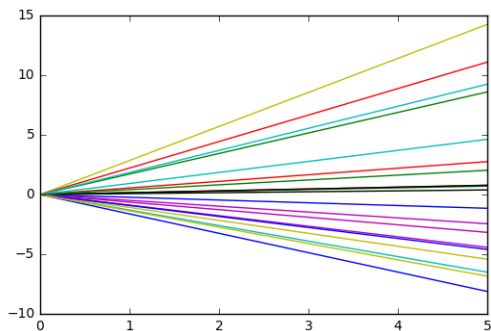
$$k(x, x') = \begin{cases} 1 & \text{if } x = x' \\ 0 & \text{otherwise} \end{cases}$$



Examples

A final example:

$$k(x, x') = xx'$$

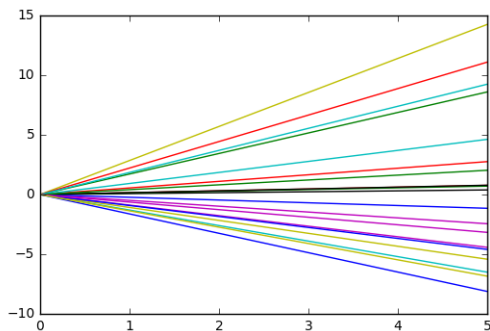


What is happening?

Examples

A final example:

$$k(x, x') = xx'$$



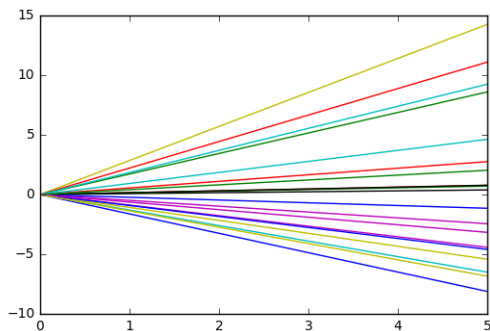
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Suppose $y(x) = cx$ where $c \sim N(0, 1)$.

Examples

A final example:

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What is happening?

Suppose $y(x) = cx$ where $c \sim N(0, 1)$.

Then
$$\begin{aligned}\text{Cov}(y(x), y(x')) &= \text{Cov}(cx, cx') = x \text{Cov}(c, c)x' \\ &= xx'\end{aligned}$$

So $y(\cdot) \sim GP(0, k(x, x'))$ with $k(x, x') = xx'$

Rules for combining covariance functions

Let k_1 and k_2 be valid covariance functions. Then

- $k_1 + k_2$ is a valid covariance function (even if k_1 and k_2 take different inputs).
- $k_1 k_2$ is a valid covariance function (also true if different inputs).
- For any function g , $k_1(g(x), g(x'))$ is a valid covariance function as is $g(x)k_1(x, x')g(x')$

Using these rules we can combine our standard set of positive definite covariance functions to create a richer family of covariance functions.

Choosing kernels and hyperparameters

GP properties are inherited primarily from the covariance function k .

- Continuity
- Differentiability
- Variance and length-scale

² f is mean square cts at x if for all sequences $x_k \rightarrow x$ we have $\mathbb{E}(f(x_k) - f(x))^2 \rightarrow 0$

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- **Variance and length-scale** controlled by hyper-parameters $k = k_\psi$:

- ▶ how much f varies between samples
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Typically choose the family of kernels by

- measures of fit (marginal likelihood, Bayes factors, ...)
- predictive skill (held-out data, cross-validation, ...)

Choose hyperparameters by maximum likelihood, Bayes, etc.

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Adler's Theorem

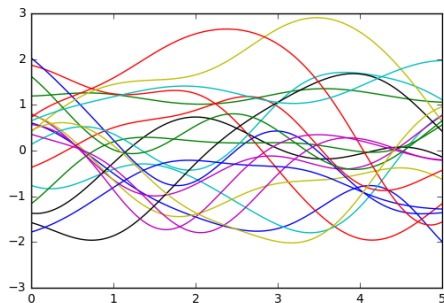
RBF/Squared-exponential/exponentiated quadratic

$$k(x, x') = \exp\left(-\frac{1}{2}(x - x')^2\right)$$

Adler's theorem gives us a way to understand the length-scale λ :

The expected number of up-crossings of u in $[0, 1]$ is

$$\frac{1}{2\pi} \sqrt{\frac{-k''(0)}{k(0)}} \exp\left(\frac{-u^2}{2k(0)}\right)$$



Adler's Theorem

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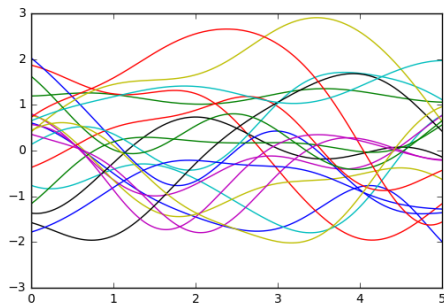
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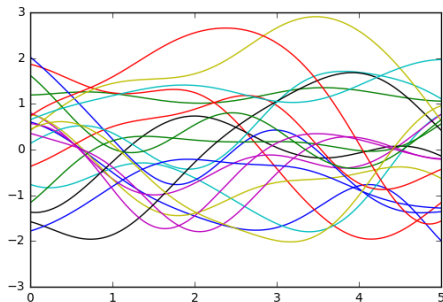
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In this random sample we have 13/17 (77%) samples crossing 0 from below.

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$$Y \sim N_d(\mu, \Sigma) \text{ if and only if } AY \sim N_p(A\mu, A\Sigma A^\top)$$

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So sums of Gaussians are Gaussian, and marginal distributions of multivariate Gaussians are still Gaussian.

Property 2: Conditional distributions are still Gaussian

Suppose

$$Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} \sim N_2(\mu, \Sigma)$$

where

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{pmatrix}$$

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Then

$$Y_2 \mid Y_1 = y_1 \sim N(\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(y_1 - \mu_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})$$

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where

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So $Y_2|Y_1 = y_1$ is Gaussian.

$$\pi(y_2|y_1) \propto \exp \left(-\frac{1}{2} \left[(y_2 - \mu_2)^\top Q_{22}(y_2 - \mu_2) + 2(y_2 - \mu_2)^\top Q_{21}(y_1 - \mu_1) \right] \right)$$

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Conditional updates of Gaussian processes

If f is a Gaussian process $f(\cdot) \sim GP(m(\cdot), k(\cdot, \cdot))$, then

$$f(x_1), \dots, f(x_n), f(x) \sim N_{n+1}(\mu, \Sigma)$$

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$$\mu = \begin{pmatrix} m(x_1) \\ \vdots \\ m(x_n) \\ m(x) \end{pmatrix} = \begin{pmatrix} | \\ m_X \\ | \\ m(x) \end{pmatrix}$$

and

$$\Sigma = \begin{pmatrix} k(x_1, x_1) & \dots & k(x_1, x_n) & k(x_1, x) \\ \vdots & & \vdots & \vdots \\ k(x_n, x_1) & \dots & k(x_n, x_n) & k(x_n, x) \\ k(x, x_1) & \dots & k(x, x_n) & k(x, x) \end{pmatrix} = \left(\begin{array}{c|c} K_{XX} & k_X(x) \\ \hline k_X(x)^\top & k(x, x) \end{array} \right)$$

where $X = \{x_1, \dots, x_n\}$, $[K_{XX}]_{ij} = k(x_i, x_j)$ is the Gram/kernel matrix,

Conditional updates of Gaussian processes

Then

$$f(x)|f(x_1), \dots, f(x_n) \sim N(\bar{m}(x), \bar{k}(x))$$

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$$\mathbf{f} = (f(x_1), \dots, f(x_n))^\top$$

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The **prior** mean and covariance functions m and k , are replaced by the **posterior** mean and covariance functions $\bar{m}$ and $\bar{k}$,

Summary: Conditional updates of Gaussian processes

If f is a Gaussian process,

$$f(\cdot) \sim GP(m(\cdot), k(\cdot, \cdot))$$

then if we observe f at $x_1, \dots, x_n$, then

$$f(\cdot) | f(x_1), \dots, f(x_n) \sim GP(\bar{m}(\cdot), \bar{k}(\cdot, \cdot))$$

where $\bar{m}$ and $\bar{k}$ are the *posterior* mean and covariance functions on the previous slide.

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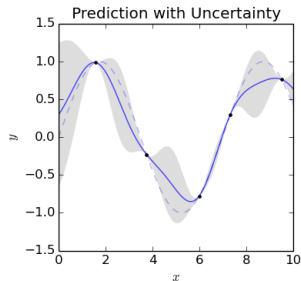
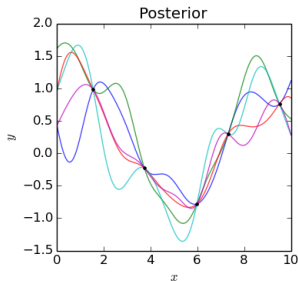
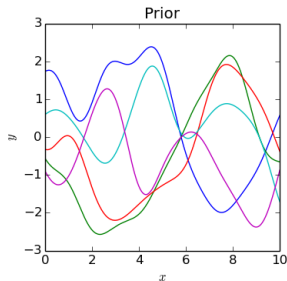
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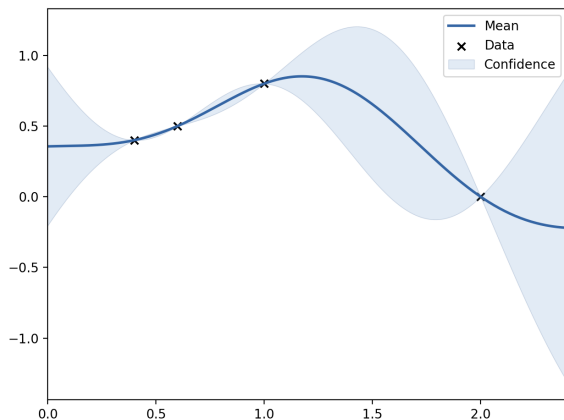
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where $\bar{m}$ and $\bar{k}$ are the *posterior* mean and covariance functions on the previous slide.

- f is still a GP even though we've observed its value at a number of locations.



No noise/*nugget* - Interpolation



Solid line $\bar{m}(x) = m(x) + k_X(x)^\top K_{XX}^{-1}(\mathbf{f} - m_X)$

Shaded region $\bar{m}(x) \pm 1.96 \sqrt{\bar{k}(x)}$

$$\bar{k}(x) = k(x, x) - k_X(x)^\top K_{XX}^{-1} k_X(x)$$

Noisy observations/with nugget - Regression

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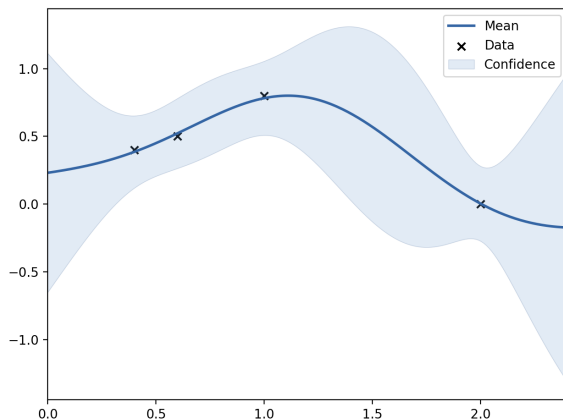
$$f(x) \mid y_1, \dots, y_n \sim N(\bar{m}(x), \bar{k}(x))$$

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Nugget standard deviation $\sigma = 0.1$

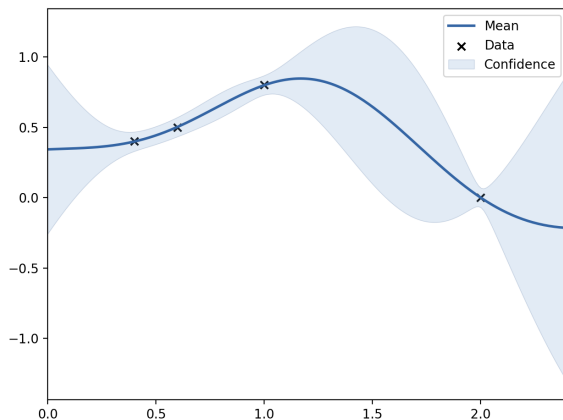


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- If

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$$y \mid D \sim \text{t-process}$$

with $n - p$ degrees of freedom.

In practice, for reasonable n , this is indistinguishable from a GP.

Why use GPs? Answer 1

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- Closed under any linear operator. If $f \sim GP(m(\cdot), k(\cdot, \cdot))$, then if $\mathcal{L}$ is a linear operator

$$\mathcal{L} \circ f \sim GP(\mathcal{L} \circ m, \mathcal{L}^2 \circ k)$$

e.g. $\frac{df}{dx}$, $\int f(x)dx$, Af are all GPs

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But the dual form only uses inner products between vectors in $\mathbb{R}^n$

$$\begin{aligned} XX^{\top} &= \begin{pmatrix} x_1^{\top} \\ \vdots \\ x_n^{\top} \end{pmatrix} (x_1 \dots x_n) = \begin{pmatrix} x_1^{\top} x_1 & \dots & x_1^{\top} x_n \\ \vdots & & \vdots \\ x_n^{\top} x_1 & \dots & x_n^{\top} x_n \end{pmatrix} \\ &= K_{XX} \text{ if } k(x, x') = x^{\top} x' \end{aligned}$$

— This is useful!

Prediction

The best prediction of y at a new location x' is

$$\begin{aligned}\hat{y}' &= x'^{\top} \hat{\beta} \\ &= x'^{\top} X^{\top} (XX^{\top} + \sigma^2 I)^{-1} y \\ &= k_X(x')^{\top} (K_{XX} + \sigma^2 I)^{-1} y\end{aligned}$$

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Note this is the GP conditional mean we derived before with $m(x) = 0$.

$$m(x) = k_X(x)^{\top} (K_{XX} + \sigma^2 I)^{-1} y$$

- linear regression and GP regression are equivalent when $k(x, x') = x^{\top} x'$.

Including features I

We can replace x by a feature vector in linear regression, e.g.,

$$\phi(x) = (1 \ x \ x^2)$$

It doesn't change the expressions other than the inner product if

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Note $k(x', x) = \phi(x')^T \phi(x)$ is a semi-definite function for any choice of $\phi(x)$.

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E.g., Consider $\mathcal{X} = \mathbb{R}^2$ and let

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So GP regression with k can be thought of as linear regression with $\phi(x)$.

Example: If $\mathcal{X} = \mathbb{R}$, set $\phi_c(x) = e^{-\frac{(x-c_0)^2}{2\lambda^2}}$ and

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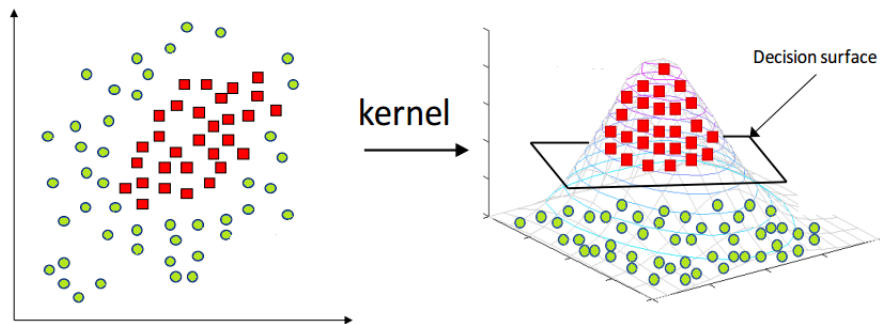
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So the RBF kernel arises when we do linear regression with an infinite feature vector containing Gaussian bumps

We can use an infinite dimensional feature vector $\phi(x)$, and because linear regression can be done solely in terms of inner-products (inverting a $n \times n$ matrix in the dual form) we never need evaluate the feature vector, only the kernel.

Kernel trick:

lift x into feature space by replacing inner products $x^\top x'$ by $k(x, x')$



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Note: $\bar{m}(\cdot) \in \mathcal{H}_k$ but samples from a GP live in a slightly larger RKHS.

TL;DR

Functions live in function spaces (vector spaces with inner products). There are lots of different function spaces: the GP kernel implicitly determines which particular (RKHS) space we work with - our hypothesis space.

- Generally, we don't think too hard about this space, we just choose a kernel and attempt to validate it empirically.

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- Generally, we don't think too hard about this space, we just choose a kernel and attempt to validate it empirically.

Although reality may not lie in the RKHS defined by k , this space is much richer than any parametric regression model³,

- thus is more likely to contain an element close to the true functional form than any class of models that contains only a finite number of features.

This is the motivation for non-parametric methods.

³and can be dense in some sets of continuous bounded functions

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If we only knew the expectation and variance of some random variables, X and Y , then how should we best do statistics?

It has been shown, using coherency arguments, or geometric arguments, or..., that the best second-order inference we can do is to update our beliefs about X given Y using

$$\mathbb{E}(X|Y) = \mathbb{E}(X) + \text{Cov}(X, Y)\text{Var}(Y)^{-1}(Y - \mathbb{E}(Y))$$

i.e., exactly the Gaussian process update for the posterior mean.

So GPs are in some sense second-order optimal.

Kriging

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Suppose $Y(x)$ is a (second order stationary) stochastic process with

$$\begin{aligned}\mathbb{E}Y(x) &= \mu \quad \forall x \\ \text{Cov}(Y(x), Y(x')) &= k(x - x') \quad \forall x, x'\end{aligned}$$

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If someone tells you $\mathbf{y} = (Y(x_1), \dots, Y(x_n))^\top$, how would you predict $Y(x)$?

One option is to find the best linear unbiased predictor (BLUP) of $Y(x)$.

Best Linear Unbiased Predictors (BLUP)

Consider the linear estimator

$$\hat{Y}(x) = c + \sum w_i Y(x_i) = c + \mathbf{w}^\top \mathbf{y}$$

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where $\boldsymbol{\mu} = (\mu, \dots, \mu)^\top$.

Thus $c = \mu - \mathbf{w}^\top \boldsymbol{\mu}$ and we must have

$$\hat{Y}(x) = \mu + \mathbf{w}^\top (\mathbf{y} - \boldsymbol{\mu})$$

Best Linear Unbiased Predictors (BLUP) - II

The **best** linear unbiased predictor minimises the mean square error

$$\begin{aligned}MSE(\hat{Y}(x)) &= \mathbb{E}((\hat{Y}(x) - Y(x))^2) \\&= \mathbb{E}\left((\mathbf{w}^\top(\mathbf{y} - \boldsymbol{\mu}) + (\mu - Y(x)))^2\right) \\&= \mathbf{w}^\top \mathbb{V}\text{ar}(\mathbf{y})\mathbf{w} + \mathbb{V}\text{ar}(Y(x)) - 2\mathbf{w}^\top \mathbb{C}\text{ov}(\mathbf{y}, Y(x)) \\&= \mathbf{w}^\top K_{XX}\mathbf{w} + k(0) - 2\mathbf{w}^\top \mathbf{k}_X(x)\end{aligned}$$

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and thus

$$\hat{Y}(x) = \mu + \mathbf{k}_X(x)^\top K_{XX}^{-1}(\mathbf{y} - \boldsymbol{\mu})$$

as before.

So the Gaussian process posterior mean is optimal (i.e. is the BLUP) even if we don't assume Gaussianity.

Why use GPs? Answer 4: Uncertainty estimates

GP predictions consist of two parts:

- point estimate $m(x) = \mathbb{E}f(x)$
- uncertainty about the estimate $k(x, x) = \text{Var}f(x)$

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Warning: the uncertainty estimates from a GP can be flawed. Note that given data $D = \{X, y\}$

$$\text{Var}(f(x)|X, y) = k(x, x) - k_X(x)K_{XX}^{-1}k_X(x)$$

The posterior variance of $f(x)$ does not directly depend upon y !

Variance estimates are particularly sensitive to the hyper-parameter estimates.

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- We pick a covariance function from a small set, based usually on differentiability considerations.
- Possibly try a few (plus combinations of a few), and use empirical evaluation to make a good choice.
- Covariance functions often contain hyper-parameters. E.g.
 - ▶ RBF kernel

$$k(x, x') = \sigma^2 \exp\left(-\frac{1}{2} \frac{(x - x')^2}{\lambda^2}\right)$$

Estimate these using your favourite statistical procedure

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E.g. consider a zero mean GP on $[0, 1]$ with covariance function

$$k(x, x') = \sigma^2 \exp(-\kappa^2 |x - x'|)$$

We can consistently estimate $\sigma^2 \kappa$, but not σ^2 or κ , even as $n \rightarrow \infty$.

Problems with hyper-parameter optimization

The likelihood surface that is maximized in hyper-parameter estimation is often flat and multi-modal,

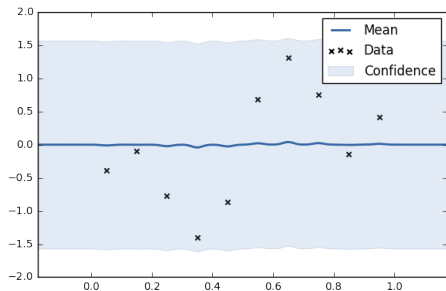
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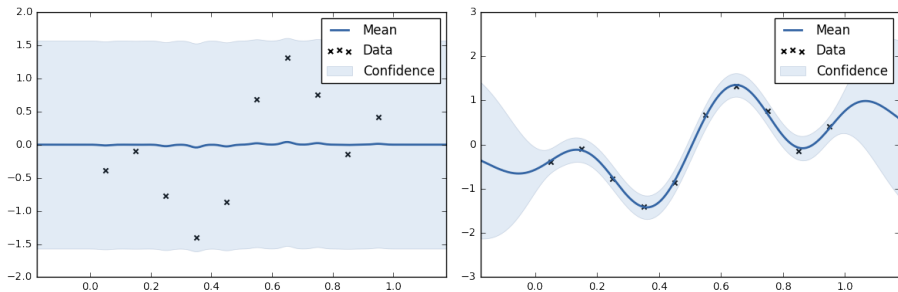


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Work around these problems by running the optimizer multiple times from random start points, using prior distributions, constraining or fixing hyper-parameters, or adding white noise.

Computational cost

The computational cost of GP training is $O(n^3)$ with $O(n^2)$ memory requirements

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Suppose

$$k(x, x') = \sum_{i=1}^m \phi_i(x) \phi_i(x') = \phi(x)^\top \phi(x')$$

Then GP regression is equivalent to linear regression with covariates $\phi(x)$

- Dual form for regression coefficients costs $O(n^3)$,
but primal solution only costs $O(m^3)$

In practice we may use a basis expansion with $m \ll n$ such that

$$k(x, x') \approx \sum_{i=1}^m \phi_i(x) \phi_i(x')$$

Choice of basis

There are many choices of basis. Two examples:

- **Mercer basis:** Consider the map

$$T_k(f)(\cdot) = \int_{\mathcal{X}} k(x, \cdot) f(x) dx$$

Consider the eigenfunctions of this map, i.e., $\phi : \mathcal{X} \mapsto \mathbb{R}$ s.t.
 $T_k(\phi)(\cdot) = \lambda \phi(\cdot)$. Mercer's theorem says that

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The Karhunen-Loeve thm says we can write $f(\cdot) \sim GP(0, k(\cdot, \cdot))$ as

$$f(x) = \sum_{i=1}^{\infty} Z_i \sqrt{\lambda_i} \phi_i(x) \quad \text{where } Z_i \stackrel{iid}{\sim} N(0, 1)$$

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We can approximate the process (& reduce cost to $O(m^3)$) by truncating the sum

$$f(x) = \sum_{i=1}^m Z_i \sqrt{\lambda_i} \phi_i(x)$$

The Mercer/KL basis minimizes the mean square truncation error. 

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Bochner's theorem says that a stationary kernel can be represented as a Fourier transform of some distribution p

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$$\begin{aligned} k(x - x') &= \int \exp(iw^\top (x - x')) p(w) dw = \mathbb{E}_{w \sim p} \exp(iw^\top (x - x')) \\ &\approx \frac{1}{m} \sum_{i=1}^m (\cos(w_i^\top x), \sin(w_i^\top x)) \begin{pmatrix} \cos(w_i^\top x') \\ \sin(w_i^\top x') \end{pmatrix} \text{ if } w_i \sim p(\cdot) \end{aligned}$$

by using Euler's identity and discarding the imaginary part.

This again reduces the complexity to $O(m^3)$.

Conclusions

- GPs are now ubiquitous in statistics/ML.
- Popularity stems from
 - ▶ Naturalness of the framework
 - ▶ Mathematical tractability
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Thank you for listening!

References

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